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Institute for Molecular Physics

University of Maryland

College Park, Maryland

E. A. Mason

J. T. Vanderslice

Statement of Research - The ultimate aim of all work of this sort is to be able to predict and correlate important properties of gases, especially at high temperatures. It is convenient to classify our work into three categories corresponding to three levels of the problem, starting from the molecular level.

(a) Intermolecular Forces. We have finished a study of the nonadditivity of three-body forces, and the manuscript is about to be submitted for publication. The third virial coefficient is a tempting quantity to investigate for nonadditivity effects, since it involves only three particles and can be measured experimentally. We first developed a model for nonadditive three-body forces and then used it to investigate the behavior of the third virial coefficient. The effects were found to be non-negligible, but unfortunately were rather dependent on the model assumed for the two-body forces. Our major conclusion was thus that further knowledge of three-body forces appears contingent on improvement in the existing knowledge of two-body forces.

Munn and Smith have collaborated in a detailed study of the interaction potential of the inert gases, based on their machine program for the rapid calculation of transport properties. This is scheduled for publication.

In collaboration with Professors I. Amdur and I. Oppenheim of M.I.T., we undertook an analysis of some of the transport properties of hydrogen and deuterium to look for a difference in their intermolecular potentials which had been indicated by second

virial coefficients and polarizabilities. The analysis indicated that there is a difference in the potentials which is consistent with the difference inferred from the other measurements. This work is scheduled for publication.

(b) Atomic and Molecular Collisions. We have finally finished the computations on the rainbow scattering of molecules according to the Airy approximation, and have submitted the work for publication.

In collaboration with Professor Barry Block of the Physics Department, we derived an expression for the radiometer force (or Knudsen gauge force) which is valid over a very large pressure range. The results can be used to obtain inelastic collision cross sections (rotational relaxation times) from the details of measured radiometer forces as a function of gas pressure. This work has been submitted for publication.

(c) Transport and Other Properties. We have continued to use the Smith-Munn machine program for calculating collision integrals for interesting models of intermolecular forces. A short note has been accepted for publication, on collision integrals for the repulsive screened Coulomb potential. We have also finished calculations of collision integrals for molecules with permanent quadrupole moments (12-6-5 potential) and for the general attractive or repulsive screened Coulomb (Debye-Hückel) potential. This last will be useful in our study of transport properties in partially ionized gases, which is now in progress. We have not yet had time

to analyze any of these calculations in detail, however, and to prepare anything for publication.

A summer student on leave from his permanent position in the Cryogenics Division of NBS, Boulder, D.E. Diller, used our quantum-mechanical collision integrals to make a complete phase-shift calculation of the low-temperature transport properties of H_2 , D_2 , and HD. This work is still being written up.

Publications - During the last six months, the following papers have appeared in the scientific literature:

HEAT CONDUCTIVITY OF POLYATOMIC AND POLAR GASES AND GAS MIXTURES. L. Monchick, A.N.G. Pereira, and E.A. Mason, J. Chem. Phys. 42, 3241(1 May 1965).

HIGHER-ORDER STATIONARY PHASE APPROXIMATIONS IN SEMICLASSICAL SCATTERING. F.J. Smith, E.A. Mason, and J.T. Vanderslice, J. Chem. Phys. 42, 3257(1 May 1965).

COLLISION INTEGRALS FOR THE EXPONENTIAL ATTRACTIVE POTENTIAL. R.J. Munn, E.A. Mason, and F.J. Smith, Phys. Fluids 8, 1103 (June 1965).

VIRIAL COEFFICIENTS FOR THE EXPONENTIAL REPULSIVE POTENTIAL. A.E. Sherwood and E.A. Mason, Phys. Fluids 8, 1577(September 1965).

In addition to the above published papers, the following have been accepted or submitted, but have not yet appeared in print:

CLASSICAL COLLISION INTEGRALS FOR THE REPULSIVE SCREENED COULOMB POTENTIAL. F.J. Smith, E.A. Mason, and R.J. Munn, Phys. Fluids 8 (scheduled for October 1965).

INTERACTION POTENTIAL OF THE INERT GASES. II. R.J. Munn and F.J. Smith, J. Chem. Phys. 42 (scheduled for December 1965).

DIFFERENCES IN THE SPHERICAL INTERMOLECULAR POTENTIALS OF HYDROGEN AND DEUTERIUM. E.A. Mason, I. Amdur, and I. Oppenheim, J. Chem. Phys. 42 (scheduled for 15 December 1965).

MOLECULAR INELASTIC COLLISION CROSS SECTIONS FROM THE RADIOMETER FORCE. E.A. Mason and B. Block, submitted to Ann. Physics (N.Y.).

MOLECULAR RAINBOWS FOR THE 12-6 POTENTIAL IN THE AIRY APPROXIMATION. E.A. Mason, R.J. Munn, and F.J. Smith, submitted to J. Chem. Phys.

NONADDITIVITY OF INTERMOLECULAR FORCES: EFFECTS ON THE THIRD VIRIAL COEFFICIENT. A.E. Sherwood, A.G. De Rocco, and E.A. Mason, J. Chem. Phys. (to be submitted).

Personnel - Dr. A.E. Sherwood left in July to accept a permanent position at the Lawrence Radiation Laboratory at Livermore. Dr. W.S. Magee, who was to have begun here as a postdoctoral research associate in September, was needed to fill an unexpected permanent opening in the Chemistry Department at Dartmouth caused by a sudden death on their faculty. We were asked by Dartmouth to release Dr. Magee from his commitment here, which we were glad to do. This throws our research plans for work on transport in very high temperature gases slightly off schedule, but not seriously. Dr. Carl Nyeland is expected to arrive from the University of Copenhagen, Denmark, in January, and is planning to work on the problem of collisions involving an atom in an electronically excited state, and the problem of excitation exchange.

There are two visitors here at present whose interests are such that they may wish to work on problems relevant to the present grant. Professor T.S. Storvick is on sabbatical leave from the Chemical Engineering Department of the University of Missouri. His interests are in equilibrium and transport properties of fluids. Dr. T.H. Spurling has a grant from the Australian government to spend a year here. His interests are intermolecular forces and

statistical mechanics.

Graduate students are also working on research problems connected with the present grant, although none of them is currently drawing any salary from it. Mr. D.E. Diller, who has already been mentioned, worked this past summer on research here, after classes were finished. Mr. J.W. Meriwether is planning work on some problems in the theory of partially ionized gases for his thesis. He is a Ph.D. candidate in chemical physics and is supported this year by a fellowship. Mr. G. Heiche has begun work on a full phase-shift calculation of mobility and charge exchange cross sections for ions in gases. He is a Ph.D. candidate in physics, and is employed at the U.S. Naval Ordnance Laboratory.